

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 317 °C

Global applicability domain: Inside

Local applicability domain index: 2.10e-01

Confidence level: 4.65e-01

Nearest Neighbors from the Training Set

Image not found

Benzoic acid, 2-benzoyl-

Measured: 261

Predicted: 309

Image not found

Benzoic acid, 2-phenoxy-

Measured: 355

Predicted: 325

Image not found

2-Acetylaminofluorene

Measured: 303

Predicted: 340

Image not found

2-Acetamidobiphenyl

Measured: 355

Predicted: 321

Image not found

Carbaryl

Measured: 315

Predicted: 297